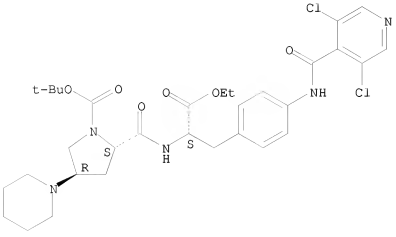
=> S L12

L13 1 L12

=> d abs fbib hitstr

L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN
AB Extremely potent very late antigen-4 (VLA-4) antagonists with picomolar, whole blood activity and slow dissociation rates were discovered by incorporating an amino substituent on the proline fragment of the initial lead structure. This level of potency against the unactivated form of VLA-4 was shown to be sufficient to overcome the poor pharmacokinetic profiles typical of this class of VLA-4 antagonists, and sustained activity as measured by receptor occupancy was achieved in preclin. species after oral dosing.
AN 2009:591429 CAPLUS
DN 151:48494
TI Discovery of N-{N-[(3-Cyanophenyl)sulfonyl]-4(R)-cyclobutylamino-(L)-prolyl}-4-[(3',5'-dichloroisonicotinoyl)amino]-(L)-phenylalanine (MK-0668), an Extremely Potent and Orally Active Antagonist of Very Late Antigen-4
AU Lin, Linus S.; Lanza, Thomas; Jewell, James P.; Liu, Ping; Jones, Carrie; Kieczykowski, Gerard R.; Treonze, Kelly; Si, Qian; Manior, Salony; Koo, Gloria; Tong, Xinchun; Wang, Junying; Schuelke, Anne; Pivnichny, James; Wang, Regina; Raab, Conrad; Vincent, Stella; Davies, Philip; MacCoss, Malcolm; Mumford, Richard A.; Hagmann, William K.
CS Departments of Medicinal Chemistry, Immunology and Rheumatology and Drug Metabolism, Merck Research Laboratories, Rahway, NJ, 07065, USA
SO Journal of Medicinal Chemistry (2009), 52(11), 3449-3452
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
IT 1160824-72-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(oral VLA-4 antagonists preparation)
RN 1160824-72-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 12:11:23 ON 28 JUL 2009)

FILE 'REGISTRY' ENTERED AT 12:11:42 ON 28 JUL 2009
L1 STRUCTURE UPLOADED
L2 32 S L1
L3 27820 S L1 FUL

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L5 3981 S L4 FUL
L6 STRUCTURE UPLOADED
L7 0 S L6
L8 18 S L6 FUL

FILE 'REGISTRY' ENTERED AT 12:16:53 ON 28 JUL 2009
L9 STRUCTURE UPLOADED
L10 0 S L9
L11 3 S L9 FUL

FILE 'REGISTRY' ENTERED AT 12:19:31 ON 28 JUL 2009
SET TERMSET E#
DEL SEL Y
SEL L11 3 RN
L12 1 S E1/RN
SET TERMSET LOGIN

FILE 'CAPLUS' ENTERED AT 12:19:43 ON 28 JUL 2009
L13 1 S L12

=> s l8
L14 2 L8

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=> s l14 not l13
L15          2 L14 NOT L13

=> d abs fbib hitstr 1-2

L15  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2009 ACS on STN
GI
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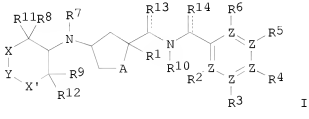

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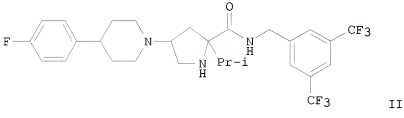

II

AB The invention relates to amino heterocyclic compds., e.g., I [Z is C or N, where no more than three Z are N; A is O, NH or substituted imino, S, SO, SO2; Y is any group given for A, acylalkyl, CO, etc.; X, X' are independently null or (un)substituted methylene or ethylene; R1-R9 are (un)substituted alkyl; R10 is H, Ph, (un)substituted alkyl; R11, R12 are independently H, acyl, OH, (un)substituted alkyl; R13, R14 are independently :O, H, Ph, (un)substituted alkyl (some of the R groups may combine to form rings)] and their pharmaceutically-acceptable salts and individual diastereomers, which are modulators of chemokine receptor activity and are useful in the prevention and treatment of inflammatory, immunoregulatory, and other diseases. Thus, compound II (two isomers) was prepared by a multistep procedure starting with the reaction of N-(tert-butoxycarbonyl)-L-valine Me ester with 3-chloro-2-(chloromethyl)-1-propene.

```
AN   2005:962240  CAPLUS
DN   143:230188
TI   Preparation of aminoprolinamide derivatives and related amino heterocycles
     as modulators of chemokine receptor activity
IN   Yang, Lihu; Pasternak, Alexander; Mills, Sander G.
PA   Merck & Co., Inc., USA
SO   PCT Int. Appl., 100 pp.
     CODEN: PIXXD2
DT   Patent
```

LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005080371	A1	20050901	WO 2005-US3849	20050208
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
				US 2004-544763P	P 20040212
	AU 2005214319	A1	20050901	AU 2005-214319	20050208
	AU 2005214319	B2	20090219		
				US 2004-544763P	P 20040212
				WO 2005-US3849	W 20050208
	CA 2555073	A1	20050901	CA 2005-2555073	20050208
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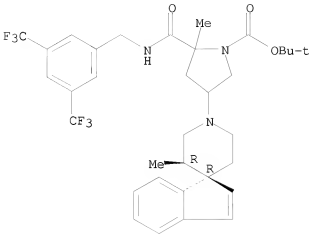
				WO 2005-US3849	W 20050208
	EP 1716134	A1	20061102	EP 2005-722806	20050208
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
				US 2004-544763P	P 20040212
				WO 2005-US3849	W 20050208
	CN 1918145	A	20070221	CN 2005-80004643	20050208
				US 2004-544763P	P 20040212
				WO 2005-US3849	W 20050208
	JP 2007522219	T	20070809	JP 2006-553179	20050208
				US 2004-544763P	P 20040212
				WO 2005-US3849	W 20050208
	IN 2006DN04625	A	20070824	IN 2006-DN4625	20060810
				US 2004-544763P	P 20040212
				WO 2005-US3849	W 20050208
	US 20070149529	A1	20070628	US 2006-589406	20060811
				US 2004-544763P	P 20040212
				WO 2005-US3849	W 20050208

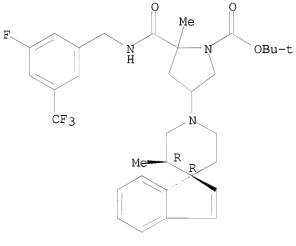
OS CASREACT 143:230188; MARPAT 143:230188
IT 862997-55-5P 862997-61-3P 862997-62-4P
862997-63-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of aminoprolinamide derivs. and related amino heterocycles as modulators of chemokine receptor activity)
RN 862997-55-5 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]carbonyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



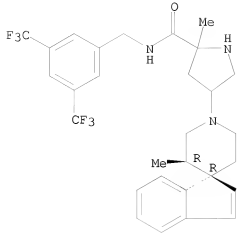
RN 862997-61-3 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[[[3-fluoro-5-(trifluoromethyl)phenyl]methyl]amino]carbonyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 862997-62-4 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]-, hydrochloride (1:1) (CA INDEX NAME)

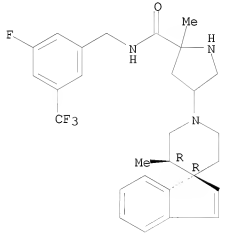
Absolute stereochemistry.



● HCl

RN 862997-63-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[[3-fluoro-5-(trifluoromethyl)phenyl]methyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]-, hydrochloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

IT 862997-29-3P 862997-33-9P 862997-51-1P
862997-64-6P 862997-65-7P 862997-66-8P
862997-68-0P 862997-69-1P 862997-82-8P

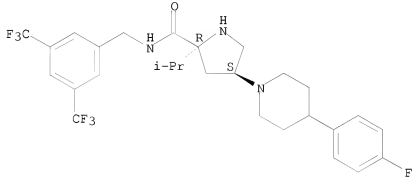
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminoprolinamide derivs. and related amino heterocycles as modulators of chemokine receptor activity)

RN 862997-29-3 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-4-[4-(4-fluorophenyl)-1-piperidinyl]-2-(1-methylethyl)-, (2R,4S)-rel-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 862997-28-2
CMF C28 H32 F7 N3 O

Relative stereochemistry.



CM 2

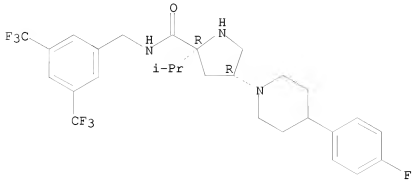
CRN 76-05-1
CMF C2 H F3 O2

RN 862997-33-9 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-4-[4-(4-fluorophenyl)-1-piperidinyl]-2-(1-methylethyl)-, (2R,4R)-rel-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 862997-32-8
CMF C28 H32 F7 N3 O

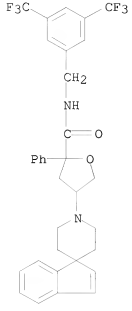
Relative stereochemistry.



CM 2

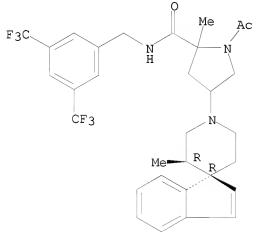
CRN 76-05-1
CMF C2 H F3 O2

RN 862997-51-1 CAPLUS
CN Pentonamide, 2,5-anhydro-N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-3,4-dideoxy-4-spiro[1H-indene-1,4'-piperidin]-1'-yl-2-C-phenyl- (9CI) (CA INDEX NAME)



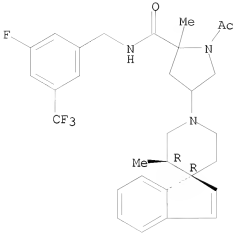
RN 862997-64-6 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-acetyl-N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]- (CA INDEX NAME)

Absolute stereochemistry.

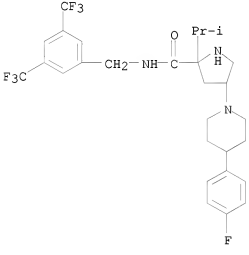


RN 862997-65-7 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-acetyl-N-[[3-fluoro-5-(trifluoromethyl)phenyl]methyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]- (CA INDEX NAME)

Absolute stereochemistry.

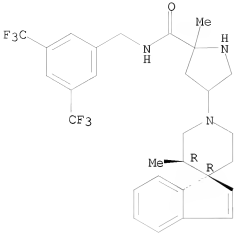


RN 862997-66-8 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-4-[4-(4-fluorophenyl)-1-piperidinyl]-2-(1-methylethyl)- (CA INDEX NAME)



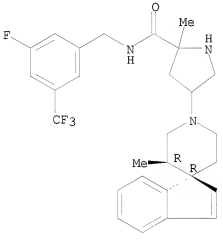
RN 862997-68-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]- (CA INDEX NAME)

Absolute stereochemistry.



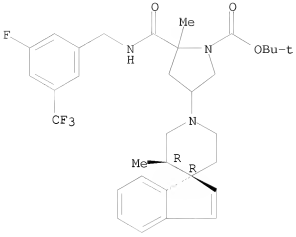
RN 862997-69-1 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[[3-fluoro-5-(trifluoromethyl)phenyl]methyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 862997-82-8 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[[[3-fluoro-5-(trifluoromethyl)phenyl]methyl]amino]carbonyl]-2-methyl-4-[(1R,3'R)-3'-methylspiro[1H-indene-1,4'-piperidin]-1'-yl]-, 1,1-dimethylethyl ester, hydrochloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.



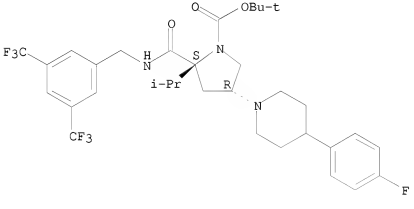
● HCl

IT 862997-39-5P 862997-40-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminoprolinamide derivs. and related amino heterocycles as modulators of chemokine receptor activity)

RN 862997-39-5 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]carbonyl]-4-[4-(4-fluorophenyl)-1-piperidinyl]-2-(1-methylethyl)-, 1,1-dimethylethyl ester, (2R,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

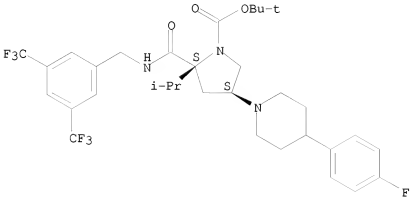


RN 862997-40-8 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]carbonyl]-4-[4-(4-fluorophenyl)-1-piperidinyl]-2-(1-methylethyl)-, 1,1-dimethylethyl ester, (2R,4R)-rel-

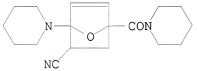
(CA INDEX NAME)

Relative stereochemistry.



OSC.G 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

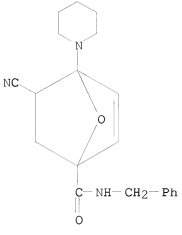
L15 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
GI



I

AB The scope of cycloaddn. reaction of various dienophiles with 5-amino-2-furancarboxamides has been studied. CH2:CHCN reacts with 5-piperidino-2-furancarboxamides, e.g. I, to yield the expected cycloaddn. products. Several other dienophiles were unreactive.
AN 1990:198001 CAPLUS
DN 112:198001
OREF 112:33465a,33468a
TI Chemistry of furan. Part VII. Diels-Alder reaction on substituted furanamides
AU Rai, Usha Kumari; Shanker, Birja; Singh, Sujan; Rao, R. Balaji
CS Dep. Chem., Banaras Hindu Univ., Varanasi, 221 005, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1989), 28B(10), 870-1
CODEN: IJSBDB; ISSN: 0376-4699
DT Journal
LA English
OS CASREACT 112:198001
IT 126774-31-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 126774-31-0 CAPLUS
CN 7-Oxabicyclo[2.2.1]hept-2-ene-1-carboxamide,
5-cyano-N-(phenylmethyl)-4-(1-piperidinyl)- (CA INDEX NAME)



OSC.G 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)